Resource Department

GEOCHEMISTRY DEPARTMENT

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ESD's Geochemistry Department has expertise in isotopic geochemistry, reactive transport modeling, experimental mineral-water kinetics, molecular geochemistry and nanogeoscience, soil geochemistry, marine geochemistry, global and regional climate modeling, and mineralogy. The department has four major thrust areas, as described below.

MOLECULAR GEOCHEMISTRY AND NANOGEOSCIENCE

This effort involves fundamental studies on the nature of the aqueous solution/mineral interface, the structure of solvated ions and colloids down to the nanometer scale, and the properties and aggregation behavior of nanoparticles. Current work includes: molecular-dynamics modeling of the interlayer-solvated cations in clays, the aggregation dynamics of nanoparticle iron oxides, and the structure of mineral interface water; studies of the solvation environment of contaminant and nutrient molecules in aqueous solution; determination of the molecular identity and kinetics of formation of iron oxide precipitates on quartz surfaces; and characterization of the surface chemistry and structure of environmentally important minerals using simulation, x-ray scattering, and x-ray spectroscopy. Many of the studies employ newly developed capabilities such as synchrotron x-ray grazing-incidence methods, and laser-based phase-sensitive nonlinear optical spectroscopy. Studies of the aqueous behavior of organic species on mineral surfaces and in solution, and on nanoparticle structure, are carried out at Berkeley Lab's Advanced Light Source as well as other synchrotron sites. The group also does extensive collaborative research using the National Center for Electron Microscopy (NCEM) at Berkeley Lab and takes advantage of the National Energy Research Scientific Computing (NERSC) facility (also at Berkeley Lab) as well as other computational sources for large-scale molecular dynamics and *ab initio* simulations. Kinetics studies, mainly focusing on heterogeneous precipitation reactions, are also conducted collaboratively with the National Science Foundation Environmental Molecular Science Institute (NSF EMSI) at Pennsylvania State University.

ISOTOPE GEOCHEMISTRY

The Center for Isotope Geochemistry (CIG) includes stable isotope and noble gas isotope laboratories; a soil carbon laboratory; an analytical chemistry laboratory; the Inductively Coupled Plasma Multi-Collector Magnetic Sector mass spectrometry laboratory; and a thermal-ionization mass spectrometry laboratory located on the UC Berkeley campus. There is also an affiliation with the cosmogenic isotope laboratory in UC Berkeley's Space Sciences Laboratory. The CIG facilities enable state-of-the-art characterization of all types of earth materials. The instrumentation and laboratories are an integral part of the Center's focus on new ways to use isotopic ratio methods to study fundamental earth processes, and environmental and energy problems of national interest.

Examples of current research programs are: (1) development of models that use isotopic composition data from element pairs in fluids to constrain fluid flow rates, water-mineral reaction rates, and the geometry and spacing of fractures in rock matrices; (2) development and application of noble gas isotopes as natural tracers for fluid source and movement in hydrocarbon and geothermal systems, and as induced phase-partitioning tracers for monitoring geologic sequestration of CO_2; (3) development of techniques for dating Quaternary geological events using U-Th-He; (4) use of U, N, and O isotopes to understand subsurface contamination sources; (5) geochemical monitoring and analysis of large-scale experiments simulating the effects of nuclear-waste heat generation within the proposed repository in Yucca Mountain, Nevada; (6) the use of C, N, and O isotopes to quantify *in situ* bioremediation and monitor remediation; (7) the use of carbon isotopes to quantify rates of organic carbon cycling and storage efficiency in soils, the impact of climate change on carbon cycling, and linkages between carbon, water, and nitrogen cycles; and (8) applications of hydrogen and oxygen isotopes to issues concerning the water cycle.

GEOCHEMICAL TRANSPORT

This effort involves simulation and study of coupled mineral-water-gas reactive transport in unsaturated porous media. The work covers infiltration/evaporation processes in the soil zone, reaction-transport processes in fractured rock under boiling conditions, injection of CO_2 in deep aquifers, hydrothermal alteration in geothermal systems, the controls on the rates of chemical weathering, and biogeochemical reaction networks in low-temperature environments. Although reaction-transport modeling and code development are the predominant activities, the group is also active in planning the analysis and drilling activities for underground thermal experiments, laboratory experiments focusing on the rates of water-mineral interaction, and field studies of geothermal systems and natural analogues for nuclear waste isolation. A new effort in this regard applies Lattice-Boltzmann models to reaction-transport processes at the microscopic scale. Efforts are also under way to understand the scale dependence of mineral-water reaction kinetics using pore network models. These new modeling efforts are being combined with the world's first experimental studies using engineered microfluidic reactors to determine mineral-water reaction rates directly at the pore (mm) scale.

Much of the geochemical transport work is focused on predicting thermally driven processes accompanying the proposed emplacement of high-level nuclear waste at Yucca Mountain, Nevada, and on the understanding of the evolution of the natural hydrogeochemical system. One focus of this work is on integrating the thermal-hydrologic-chemical environment in the near field of the proposed Yucca Mountain repository with THC processes occurring inside emplacement drifts, including on the surface of the waste package (where corrosion is the main issue) and inside the waste packages (where dissolution of spent fuel is the main issue). Another focus is on understanding the controls on chemical weathering. One such effort involves integration of uranium-series isotopic disequilibria with major element profiles to determine *in situ* reaction rates in deep-sea marine sediments. Another involves understanding the controls on, and rates of, formation of weathering rinds; this work has demonstrated the key role of reaction-induced porosity change in controlling the weathering rate. Collaboration with other departments in ESD brings together essential pieces of the problem, including hydrological processes in the unsaturated zone, thermodynamics and kinetics of geochemical processes, and isotopic effects.

Current projects include:

(1) Analysis of geochemical and isotopic data from Yucca Mountain to constrain models of flow and transport in the unsaturated zone
(2) Development of models for reactive-transport in unsaturated systems and co-development of the reactive-transport code TOUGHREACT
(3) Improved thermodynamic and kinetic databases for water-rock interaction modeling
(4) Research on natural analogue sites, including the Yellowstone geothermal system, Peña Blanca, Mexico, and the Idaho National Engineering and Environmental Laboratory subsurface conditions
(5) Modeling of CO_2 sequestration in saline aquifers
(6) Modeling hydrothermal alteration in geothermal systems
(7) Development of a Pitzer-type geochemical reactive transport model and simulation of high-ionic-strength groundwater contamination
(8) Prediction of the rate of strontium migration at the Hanford site
(9) Experimental and modeling studies on the scale dependence of mineral reaction kinetics
(10) Modeling of bioremediation field tests at the Hanford site
(11) Study of long-term benthic biogeochemical dynamics of heavy metal cycling and benthic fluxes in lake sediments at Lake Coeur d'Alene, Idaho, including the development of a dynamic numerical biogeochemical model of heavy metal fate and transport in benthic sediments.

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